



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2026 – 10:07 am BST

PDB ID : 9HHX / pdb_00009hhx
Title : Plant membrane receptor IGP1
Authors : Jimenez-Sandoval, P.; Santiago, J.
Deposited on : 2024-11-22
Resolution : 2.62 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

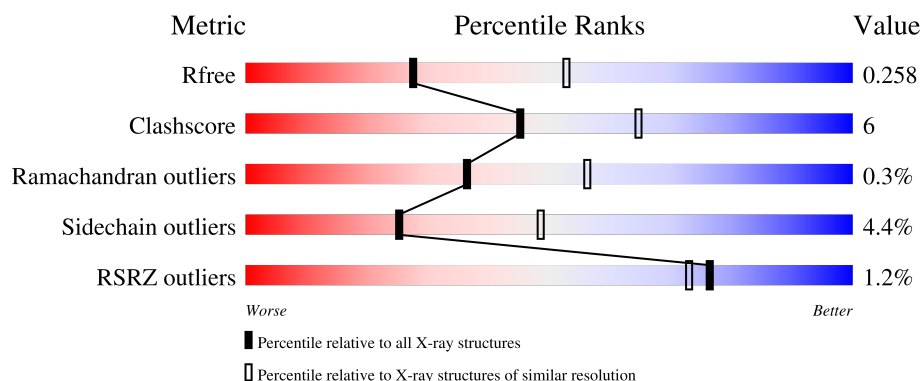
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	618	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>...</div> </div> </div>
2	B	3	<div> <div>67%</div> <div>33%</div> </div>
2	D	3	<div> <div>33%</div> <div>67%</div> </div>
3	C	6	<div> <div>100%</div> </div>
4	E	3	<div> <div>100%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4806 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

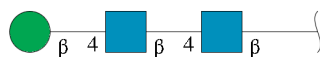
- Molecule 1 is a protein called non-specific serine/threonine protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	593	4487	2856	759	854	18	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

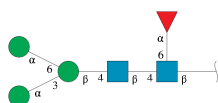
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP C0LGH4
A	24	GLY	-	expression tag	UNP C0LGH4
A	631	LEU	-	expression tag	UNP C0LGH4
A	632	GLU	-	expression tag	UNP C0LGH4
A	633	GLY	-	expression tag	UNP C0LGH4
A	634	SER	-	expression tag	UNP C0LGH4
A	635	GLU	-	expression tag	UNP C0LGH4
A	636	ASN	-	expression tag	UNP C0LGH4
A	637	LEU	-	expression tag	UNP C0LGH4
A	638	TYR	-	expression tag	UNP C0LGH4
A	639	PHE	-	expression tag	UNP C0LGH4
A	640	GLN	-	expression tag	UNP C0LGH4

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



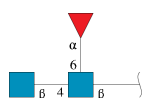
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	39	22	2	15	0	0	0
2	D	3	39	22	2	15	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



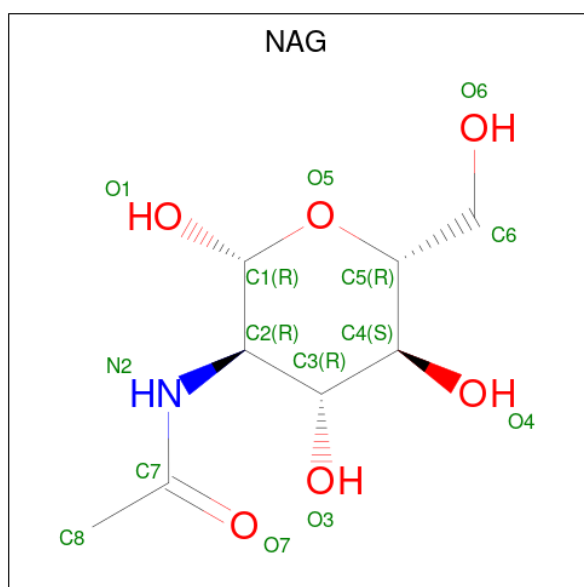
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



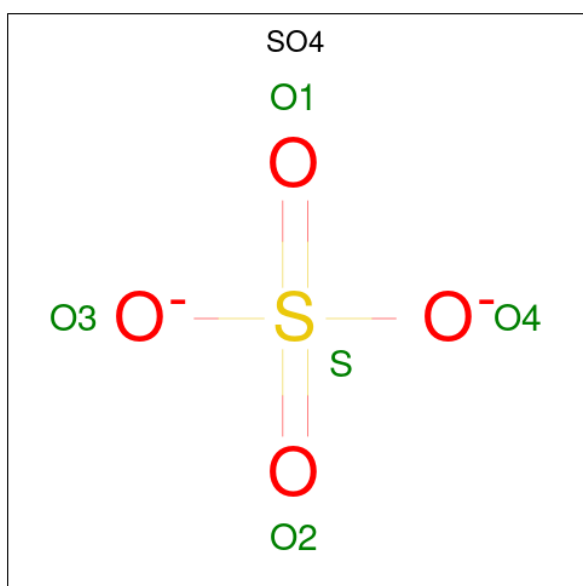
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0

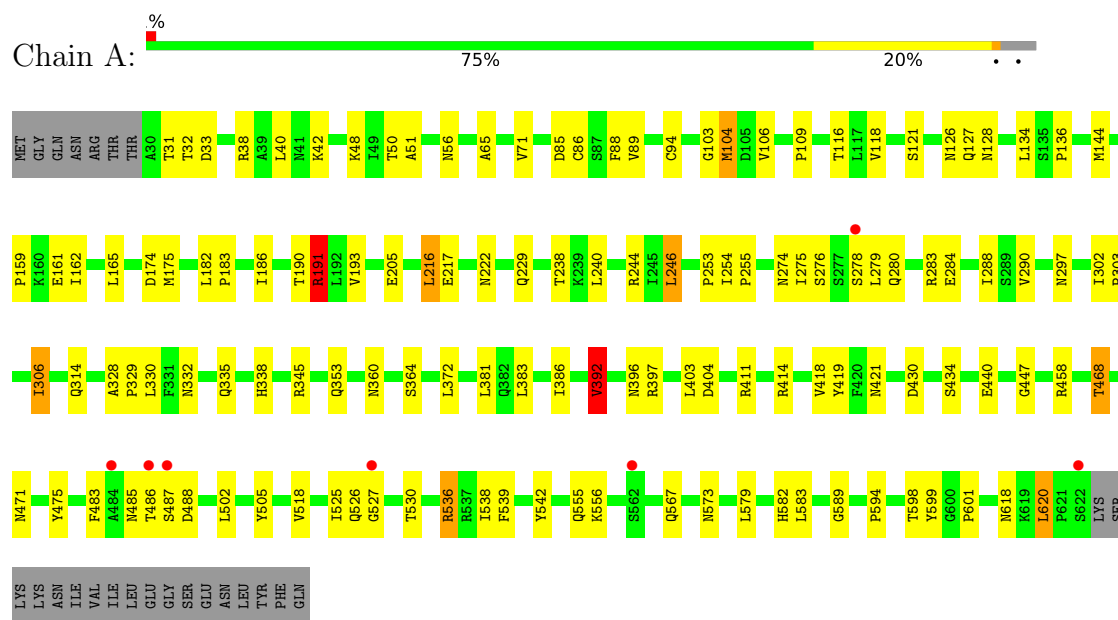
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	55	Total	O	0	0
			55	55		

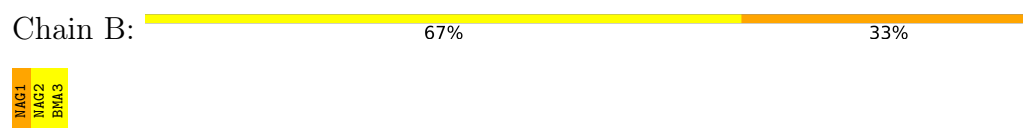
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: non-specific serine/threonine protein kinase



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose




- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

MAG1
MAG2
BGA3
MAN4
MAN5
FUC6

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	84.36Å 84.36Å 198.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.07 – 2.62 49.07 – 2.62	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.07-2.62) 100.0 (49.07-2.62)	Depositor EDS
R_{merge}	0.43	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.182 , 0.256 0.190 , 0.258	Depositor DCC
R_{free} test set	1185 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.083 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4806	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MAN, BMA, SO4, NAG, FUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.80	0/4580	1.43	34/6239 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	MET	CB-CA-C	-7.91	95.90	109.65
1	A	314	GLN	CB-CA-C	7.75	121.56	110.24
1	A	283	ARG	N-CA-CB	7.48	121.95	110.14
1	A	297	ASN	OD1-CG-ND2	-7.33	115.28	122.60
1	A	191	ARG	N-CA-CB	-6.97	100.37	110.47
1	A	430	ASP	CA-CB-CG	6.82	119.42	112.60
1	A	48	LYS	CB-CA-C	6.56	121.87	111.51
1	A	589	GLY	CA-C-O	-6.44	117.79	122.23
1	A	48	LYS	CB-CG-CD	6.42	126.08	111.30
1	A	238	THR	CA-CB-OG1	-6.37	100.05	109.60
1	A	134	LEU	N-CA-CB	-6.35	99.78	109.94
1	A	404	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	126	ASN	CB-CA-C	6.22	120.28	109.65
1	A	414	ARG	N-CA-CB	6.08	118.92	109.97
1	A	526	GLN	CB-CA-C	-6.00	99.78	113.33
1	A	38	ARG	CB-CA-C	5.90	120.58	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	GLN	N-CA-CB	-5.85	100.40	111.00
1	A	483	PHE	N-CA-CB	-5.77	103.88	110.35
1	A	38	ARG	CA-CB-CG	5.76	125.62	114.10
1	A	50	THR	CA-CB-OG1	-5.75	100.97	109.60
1	A	136	PRO	CB-CA-C	-5.65	103.83	111.85
1	A	414	ARG	CB-CG-CD	5.63	124.25	111.30
1	A	190	THR	CA-CB-OG1	-5.55	101.28	109.60
1	A	392	VAL	N-CA-CB	5.52	120.34	111.23
1	A	555	GLN	CB-CA-C	5.50	119.52	110.88
1	A	573	ASN	CB-CA-C	5.46	118.74	109.84
1	A	85	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	216	LEU	N-CA-CB	-5.23	102.17	110.06
1	A	38	ARG	N-CA-C	-5.21	105.61	111.28
1	A	161	GLU	CB-CG-CD	5.17	121.40	112.60
1	A	556	LYS	N-CA-CB	5.16	117.70	110.12
1	A	525	ILE	CB-CA-C	5.14	117.17	110.96
1	A	284	GLU	CB-CA-C	5.07	119.13	110.56
1	A	290	VAL	N-CA-CB	5.04	118.89	112.34

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	ARG	Sidechain
1	A	244	ARG	Sidechain
1	A	397	ARG	Sidechain
1	A	411	ARG	Sidechain
1	A	536	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4487	0	4365	54	0
2	B	39	0	34	4	0
2	D	39	0	34	0	0
3	C	71	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	38	0	34	0	0
5	A	56	0	52	0	0
6	A	20	0	0	2	0
7	A	1	0	0	0	0
8	A	55	0	0	3	0
All	All	4806	0	4580	55	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ALA:H	2:B:1:NAG:H81	1.31	0.92
1:A:51:ALA:N	2:B:1:NAG:H81	2.02	0.75
1:A:421:ASN:O	1:A:458:ARG:NH1	2.22	0.72
1:A:56:ASN:HD22	2:B:1:NAG:H83	1.57	0.69
1:A:542:TYR:HB2	1:A:582:HIS:HB3	1.80	0.64
1:A:222:ASN:HA	1:A:246:LEU:O	2.01	0.60
1:A:338:HIS:NE2	8:A:802:HOH:O	2.31	0.60
1:A:345:ARG:NH2	6:A:708:SO4:O1	2.32	0.59
1:A:381:LEU:HD23	1:A:383:LEU:HD22	1.84	0.59
1:A:191:ARG:NH2	6:A:706:SO4:O4	2.33	0.56
1:A:468:THR:HG22	1:A:599:TYR:OH	2.06	0.56
1:A:539:PHE:CD2	1:A:601:PRO:HA	2.43	0.54
1:A:392:VAL:HG11	1:A:403:LEU:HB3	1.90	0.54
1:A:447:GLY:HA2	1:A:475:TYR:CE1	2.43	0.53
1:A:217:GLU:HA	1:A:240:LEU:HA	1.91	0.52
1:A:527:GLY:O	1:A:530:THR:HG22	2.09	0.52
1:A:193:VAL:HA	1:A:216:LEU:HA	1.93	0.51
8:A:845:HOH:O	2:B:1:NAG:H83	2.11	0.50
1:A:229:GLN:HE21	1:A:253:PRO:HD2	1.75	0.49
1:A:40:LEU:C	1:A:40:LEU:HD13	2.37	0.49
1:A:116:THR:O	1:A:118:VAL:HG13	2.13	0.49
1:A:165:LEU:HD23	1:A:165:LEU:N	2.30	0.47
1:A:353:GLN:HA	8:A:834:HOH:O	2.14	0.47
1:A:328:ALA:N	1:A:329:PRO:HD2	2.30	0.47
1:A:278:SER:O	1:A:279:LEU:HB2	2.15	0.46
1:A:486:THR:HG22	1:A:487:SER:O	2.15	0.46
1:A:539:PHE:CE2	1:A:601:PRO:HA	2.49	0.46
1:A:288:ILE:HG23	1:A:288:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:THR:O	1:A:33:ASP:C	2.56	0.46
1:A:174:ASP:OD2	1:A:175:MET:HE2	2.15	0.46
1:A:104:MET:HE3	1:A:104:MET:HB3	1.81	0.45
1:A:594:PRO:HD2	1:A:598:THR:HG21	1.99	0.45
1:A:103:GLY:HA2	1:A:127:GLN:O	2.17	0.45
1:A:106:VAL:HG22	1:A:128:ASN:CG	2.42	0.45
1:A:86:CYS:HA	1:A:94:CYS:HA	1.99	0.45
1:A:364:SER:HA	1:A:386:ILE:O	2.17	0.44
1:A:306:ILE:HG23	1:A:330:LEU:HD13	1.98	0.44
1:A:468:THR:HG22	1:A:599:TYR:CZ	2.53	0.44
1:A:121:SER:HA	1:A:144:MET:HA	2.00	0.44
1:A:328:ALA:N	1:A:329:PRO:CD	2.81	0.44
1:A:418:VAL:HG21	1:A:620:LEU:HD23	2.00	0.43
1:A:302:ILE:O	1:A:303:PRO:C	2.61	0.43
1:A:159:PRO:O	1:A:162:ILE:HG13	2.19	0.43
1:A:579:LEU:C	1:A:579:LEU:HD23	2.44	0.43
1:A:254:ILE:HA	1:A:255:PRO:HD3	1.88	0.42
1:A:274:ASN:O	1:A:275:ILE:C	2.61	0.42
1:A:502:LEU:HD23	1:A:583:LEU:HD12	2.02	0.42
1:A:65:ALA:HB1	1:A:71:VAL:HG11	2.01	0.41
1:A:381:LEU:CD2	1:A:383:LEU:HD22	2.50	0.41
1:A:505:TYR:HA	1:A:579:LEU:O	2.20	0.41
1:A:372:LEU:HB2	1:A:396:ASN:ND2	2.36	0.41
1:A:182:LEU:HA	1:A:183:PRO:HD3	1.91	0.40
1:A:278:SER:O	1:A:279:LEU:CB	2.69	0.40
1:A:419:TYR:HA	1:A:618:ASN:HA	2.02	0.40
1:A:88:PHE:O	1:A:89:VAL:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	592/618 (96%)	551 (93%)	39 (7%)	2 (0%)	36 56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	SER
1	A	392	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	479/529 (90%)	458 (96%)	21 (4%)	25 48

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	42	LYS
1	A	109	PRO
1	A	186	ILE
1	A	205	GLU
1	A	246	LEU
1	A	280	GLN
1	A	306	ILE
1	A	332	ASN
1	A	335	GLN
1	A	360	ASN
1	A	434	SER
1	A	440	GLU
1	A	468	THR
1	A	471	ASN
1	A	485	ASN
1	A	488	ASP
1	A	518	VAL
1	A	536	ARG

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Mol	Chain	Res	Type
1	A	538	ILE
1	A	620	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	280	GLN
1	A	335	GLN
1	A	360	ASN
1	A	596	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

15 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	B	1	2,1	14,14,15	0.79	1 (7%)	17,19,21	2.01	3 (17%)
2	NAG	B	2	2	14,14,15	1.04	1 (7%)	17,19,21	2.51	7 (41%)
2	BMA	B	3	2	11,11,12	0.60	0	15,15,17	1.03	1 (6%)
3	NAG	C	1	3,1	14,14,15	1.13	2 (14%)	17,19,21	2.10	5 (29%)
3	NAG	C	2	3	14,14,15	0.66	0	17,19,21	2.26	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	C	3	3	11,11,12	0.67	0	15,15,17	1.77	3 (20%)
3	MAN	C	4	3	11,11,12	0.61	0	15,15,17	1.16	3 (20%)
3	MAN	C	5	3	11,11,12	0.63	0	15,15,17	1.29	2 (13%)
3	FUC	C	6	3	10,10,11	0.44	0	14,14,16	1.37	2 (14%)
2	NAG	D	1	2,1	14,14,15	1.03	1 (7%)	17,19,21	1.63	4 (23%)
2	NAG	D	2	2	14,14,15	0.77	0	17,19,21	1.58	1 (5%)
2	BMA	D	3	2	11,11,12	0.56	0	15,15,17	0.70	0
4	NAG	E	1	4,1	14,14,15	1.31	2 (14%)	17,19,21	2.28	6 (35%)
4	NAG	E	2	4	14,14,15	1.88	4 (28%)	17,19,21	2.06	8 (47%)
4	FUC	E	3	4	10,10,11	0.74	0	14,14,16	1.55	5 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	1/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
3	FUC	C	6	3	-	-	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	FUC	E	3	4	-	-	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	NAG	C3-C2	3.09	1.59	1.52
4	E	2	NAG	O4-C4	2.92	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	NAG	C3-C2	2.82	1.58	1.52
4	E	2	NAG	C8-C7	2.67	1.56	1.50
2	B	2	NAG	C8-C7	2.61	1.56	1.50
4	E	1	NAG	O3-C3	2.51	1.48	1.43
4	E	2	NAG	C2-N2	2.36	1.50	1.46
3	C	1	NAG	C8-C7	2.31	1.55	1.50
2	B	1	NAG	C2-N2	-2.20	1.42	1.46
2	D	1	NAG	C2-N2	-2.06	1.42	1.46
3	C	1	NAG	C4-C3	2.01	1.57	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	O7-C7-N2	-5.80	111.29	121.95
3	C	2	NAG	O5-C5-C6	5.53	115.87	107.20
3	C	3	BMA	C1-O5-C5	5.46	119.59	112.19
3	C	1	NAG	C8-C7-N2	5.37	125.19	116.10
4	E	1	NAG	C8-C7-N2	5.27	125.01	116.10
2	B	1	NAG	O3-C3-C2	-5.08	98.96	109.47
2	D	2	NAG	O5-C5-C6	-4.97	99.42	107.20
2	B	2	NAG	C4-C3-C2	-4.37	104.61	111.02
2	B	2	NAG	C8-C7-N2	4.15	123.13	116.10
2	B	1	NAG	O5-C5-C6	-4.04	100.88	107.20
2	B	1	NAG	O6-C6-C5	-3.99	97.60	111.29
4	E	1	NAG	O3-C3-C2	3.95	117.65	109.47
3	C	2	NAG	C1-O5-C5	3.91	117.49	112.19
4	E	2	NAG	C1-O5-C5	3.76	117.29	112.19
4	E	2	NAG	C2-N2-C7	3.48	127.86	122.90
3	C	1	NAG	O7-C7-C8	-3.43	115.69	122.06
2	D	1	NAG	O6-C6-C5	-3.35	99.79	111.29
3	C	2	NAG	O4-C4-C5	-3.26	101.20	109.30
3	C	1	NAG	C4-C3-C2	-3.24	106.26	111.02
3	C	2	NAG	C6-C5-C4	-3.24	105.41	113.00
4	E	1	NAG	C2-N2-C7	-3.16	118.40	122.90
4	E	3	FUC	C1-O5-C5	3.14	119.89	112.78
2	B	2	NAG	C2-N2-C7	-3.09	118.50	122.90
3	C	6	FUC	C2-C3-C4	-3.08	105.57	110.89
2	B	2	NAG	O3-C3-C4	3.07	117.44	110.35
3	C	2	NAG	C1-C2-N2	2.91	115.45	110.49
4	E	1	NAG	O7-C7-N2	-2.87	116.67	121.95
2	D	1	NAG	C1-C2-N2	-2.82	105.67	110.49
4	E	1	NAG	C4-C3-C2	-2.79	106.92	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	O3-C3-C2	-2.67	103.93	109.47
3	C	5	MAN	C1-O5-C5	2.57	115.68	112.19
2	B	3	BMA	O5-C1-C2	-2.55	106.84	110.77
3	C	4	MAN	C1-O5-C5	2.54	115.64	112.19
4	E	3	FUC	O3-C3-C2	-2.52	105.16	109.99
3	C	1	NAG	O4-C4-C3	2.50	116.13	110.35
4	E	2	NAG	O4-C4-C5	2.46	115.41	109.30
4	E	2	NAG	O4-C4-C3	2.39	115.88	110.35
3	C	1	NAG	O3-C3-C2	-2.37	104.57	109.47
3	C	4	MAN	O5-C1-C2	2.35	114.39	110.77
4	E	3	FUC	C3-C4-C5	2.34	113.42	109.77
4	E	2	NAG	O7-C7-C8	2.33	126.39	122.06
4	E	2	NAG	C1-C2-N2	2.30	114.42	110.49
2	B	2	NAG	O3-C3-C2	-2.30	104.71	109.47
4	E	2	NAG	C3-C4-C5	-2.29	106.15	110.24
3	C	2	NAG	O7-C7-C8	-2.28	117.83	122.06
3	C	4	MAN	O2-C2-C3	2.26	114.67	110.14
3	C	3	BMA	C1-C2-C3	-2.19	106.97	109.67
2	B	2	NAG	C3-C4-C5	-2.18	106.35	110.24
4	E	2	NAG	O3-C3-C2	2.14	113.89	109.47
4	E	3	FUC	C2-C3-C4	2.12	114.57	110.89
3	C	3	BMA	O2-C2-C3	2.10	114.35	110.14
3	C	6	FUC	O3-C3-C2	2.08	113.97	109.99
2	D	1	NAG	O5-C5-C6	2.05	110.42	107.20
4	E	3	FUC	O5-C5-C4	2.04	113.18	109.52
3	C	5	MAN	O3-C3-C2	-2.03	106.11	109.99
4	E	1	NAG	O7-C7-C8	-2.02	118.31	122.06

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	B	2	NAG	O7-C7-N2-C2
2	D	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2

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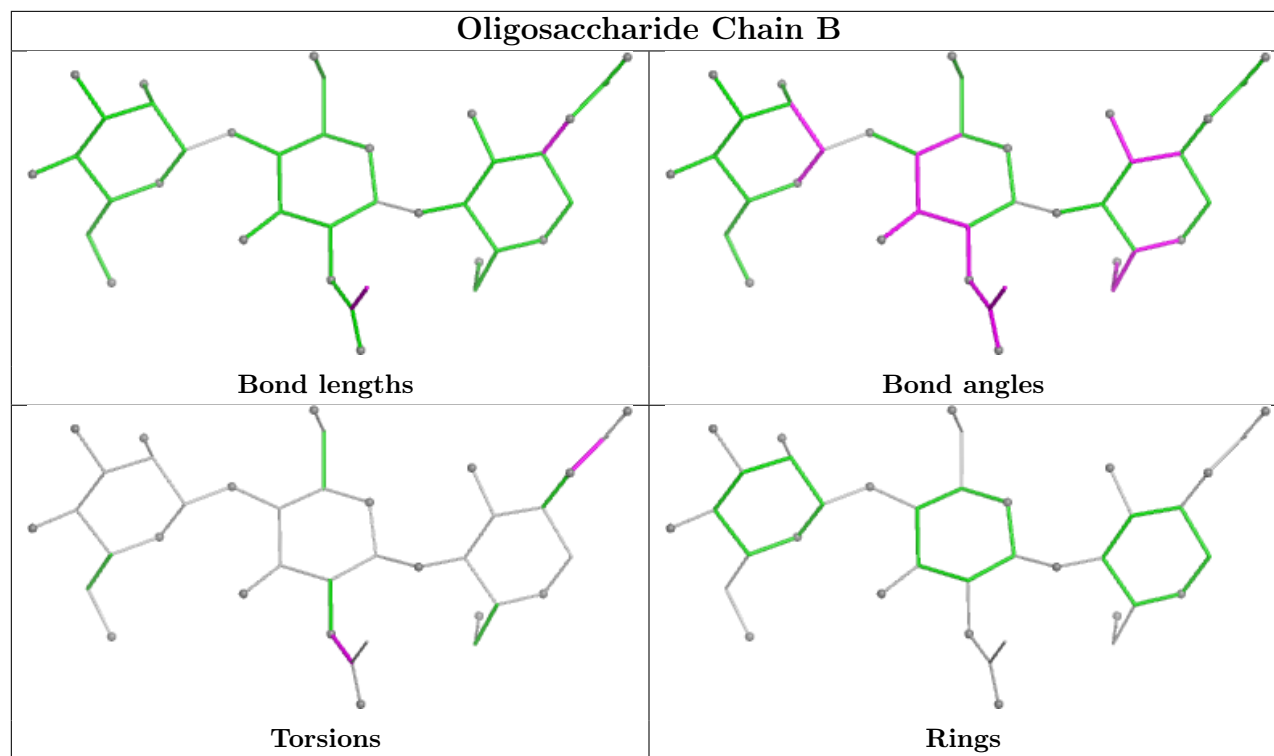
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
3	C	5	MAN	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	5	MAN	O5-C5-C6-O6

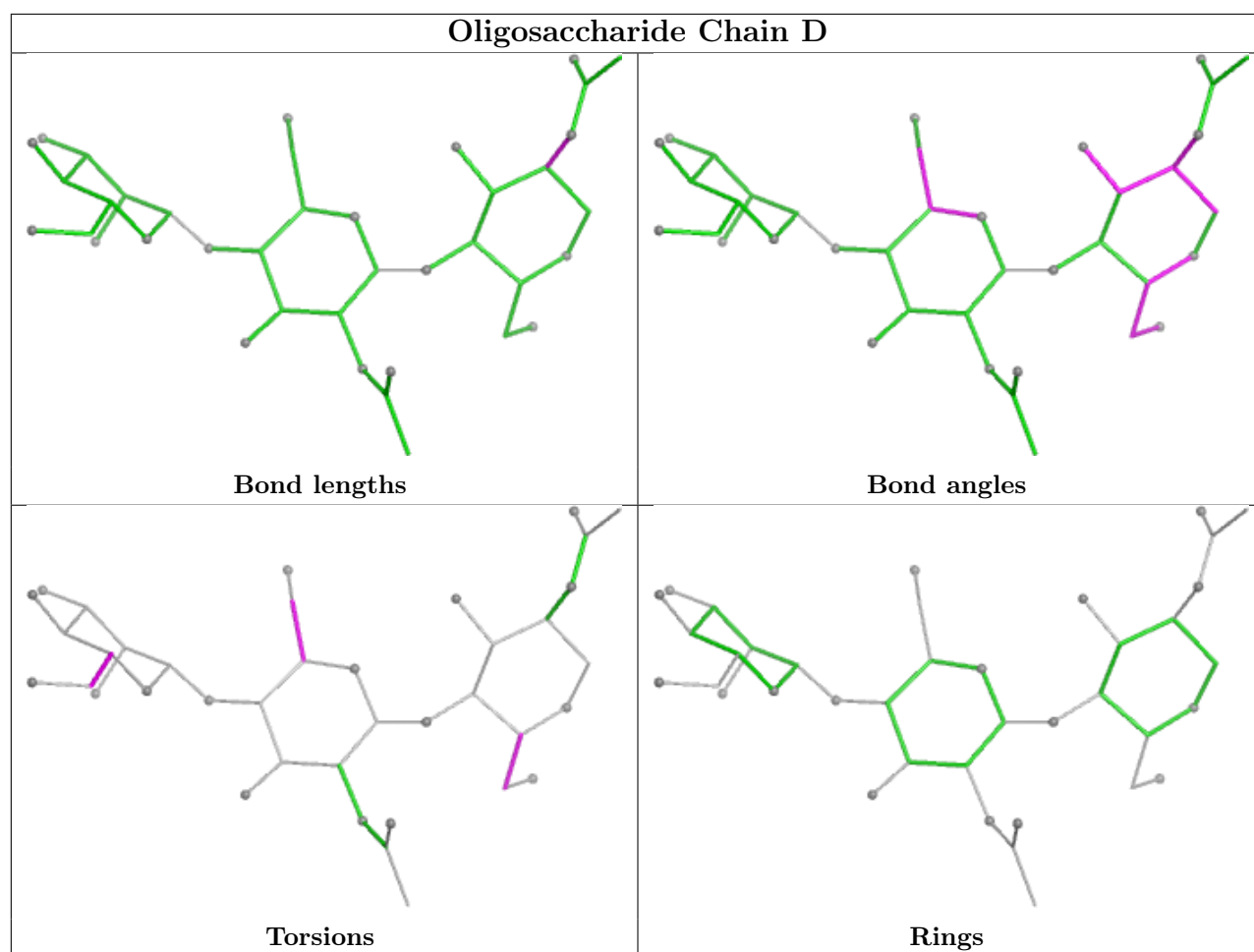
There are no ring outliers.

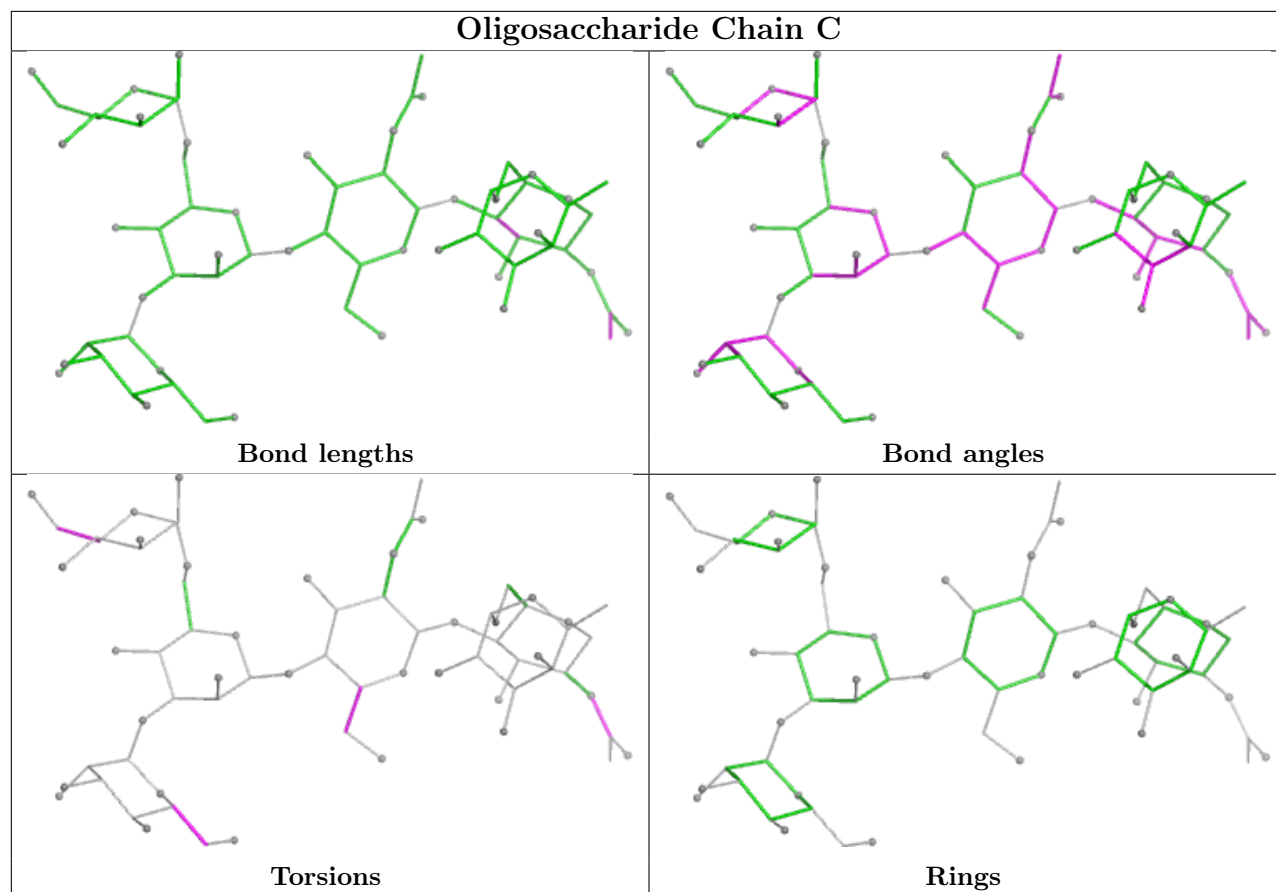
1 monomer is involved in 4 short contacts:

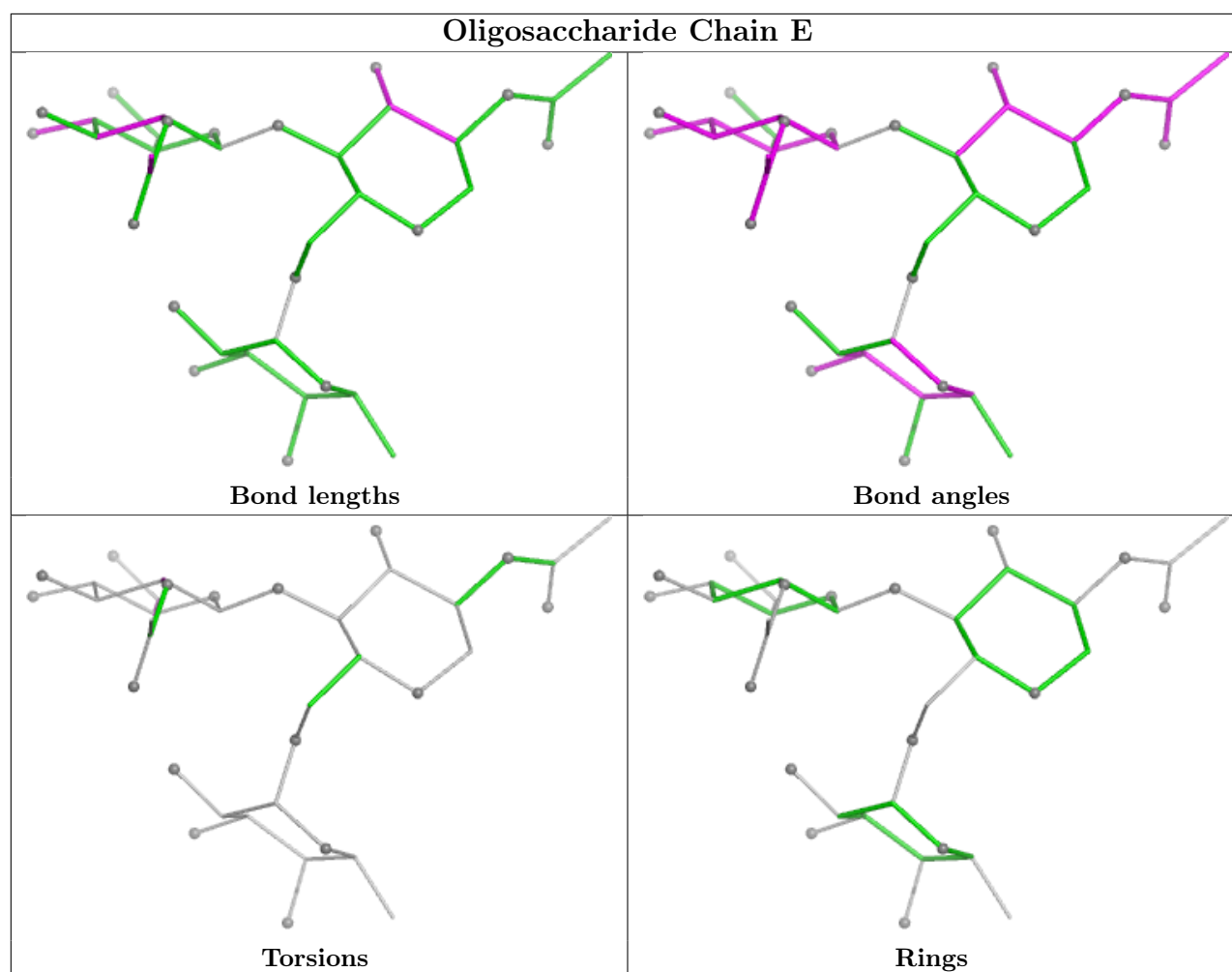
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	704	1	14,14,15	1.02	1 (7%)	17,19,21	2.70	4 (23%)
6	SO4	A	706	-	4,4,4	0.32	0	6,6,6	0.27	0
6	SO4	A	707	-	4,4,4	0.29	0	6,6,6	0.23	0
5	NAG	A	703	1	14,14,15	0.98	0	17,19,21	2.87	8 (47%)
5	NAG	A	702	1	14,14,15	0.94	1 (7%)	17,19,21	2.53	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	701	1	14,14,15	1.60	3 (21%)	17,19,21	2.76	7 (41%)
6	SO4	A	708	-	4,4,4	0.29	0	6,6,6	0.16	0
6	SO4	A	705	-	4,4,4	0.25	0	6,6,6	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	703	1	-	4/6/23/26	0/1/1/1
5	NAG	A	701	1	-	1/6/23/26	0/1/1/1
5	NAG	A	704	1	-	2/6/23/26	0/1/1/1
5	NAG	A	702	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	NAG	C4-C5	3.12	1.59	1.53
5	A	701	NAG	O4-C4	2.89	1.49	1.43
5	A	704	NAG	C2-N2	2.75	1.51	1.46
5	A	701	NAG	O5-C5	2.62	1.48	1.43
5	A	702	NAG	C8-C7	2.51	1.55	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	704	NAG	O5-C5-C6	6.28	117.05	107.20
5	A	703	NAG	O5-C5-C6	6.21	116.93	107.20
5	A	701	NAG	O4-C4-C5	5.78	123.64	109.30
5	A	702	NAG	C8-C7-N2	5.73	125.80	116.10
5	A	703	NAG	C1-O5-C5	5.55	119.71	112.19
5	A	701	NAG	C3-C4-C5	-5.45	100.51	110.24
5	A	704	NAG	C2-N2-C7	5.42	130.62	122.90
5	A	704	NAG	C1-C2-N2	4.88	118.83	110.49
5	A	701	NAG	C1-O5-C5	-4.29	106.38	112.19
5	A	703	NAG	C8-C7-N2	-4.12	109.13	116.10
5	A	704	NAG	O4-C4-C3	-3.91	101.30	110.35
5	A	701	NAG	O5-C5-C6	3.81	113.18	107.20
5	A	702	NAG	O7-C7-N2	-3.78	115.01	121.95
5	A	702	NAG	O3-C3-C4	-3.60	102.02	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	703	NAG	O4-C4-C5	3.53	118.07	109.30
5	A	703	NAG	O5-C5-C4	-3.41	102.52	110.83
5	A	701	NAG	C2-N2-C7	3.36	127.69	122.90
5	A	703	NAG	O7-C7-N2	3.29	128.00	121.95
5	A	702	NAG	O3-C3-C2	-3.12	103.01	109.47
5	A	702	NAG	C4-C3-C2	2.93	115.31	111.02
5	A	701	NAG	C4-C3-C2	2.78	115.09	111.02
5	A	703	NAG	C3-C4-C5	-2.73	105.38	110.24
5	A	702	NAG	O4-C4-C5	2.44	115.36	109.30
5	A	703	NAG	C6-C5-C4	2.41	118.66	113.00
5	A	702	NAG	C2-N2-C7	-2.39	119.50	122.90
5	A	702	NAG	O5-C5-C6	-2.33	103.55	107.20
5	A	701	NAG	C6-C5-C4	2.24	118.25	113.00

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	702	NAG	C8-C7-N2-C2
5	A	702	NAG	O7-C7-N2-C2
5	A	704	NAG	O5-C5-C6-O6
5	A	704	NAG	C4-C5-C6-O6
5	A	703	NAG	C8-C7-N2-C2
5	A	701	NAG	C4-C5-C6-O6
5	A	703	NAG	O7-C7-N2-C2
5	A	703	NAG	C4-C5-C6-O6
5	A	703	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	706	SO4	1	0
6	A	708	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	593/618 (95%)	-0.40	7 (1%) 76 73	14, 33, 57, 99	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	ALA	4.1
1	A	622	SER	3.7
1	A	487	SER	3.6
1	A	562	SER	2.9
1	A	486	THR	2.5
1	A	527	GLY	2.2
1	A	278	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

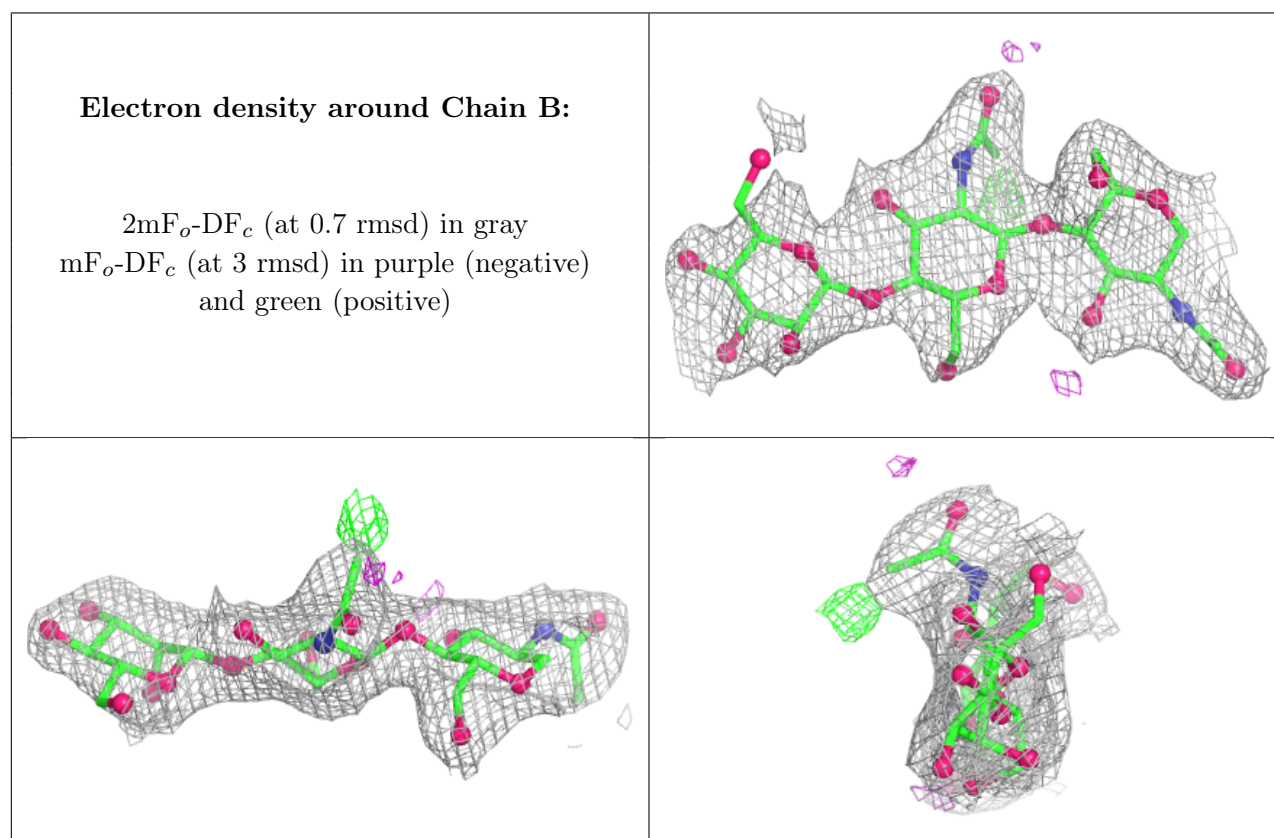
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	C	4	11/12	0.65	0.15	81,93,105,106	0
4	NAG	E	2	14/15	0.80	0.13	53,73,85,87	0
2	BMA	B	3	11/12	0.84	0.10	67,77,87,87	0
2	NAG	B	2	14/15	0.86	0.11	46,53,62,70	0
2	NAG	D	2	14/15	0.86	0.12	53,61,81,97	0

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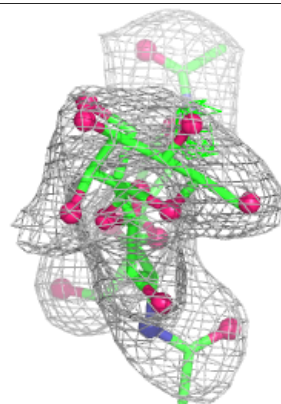
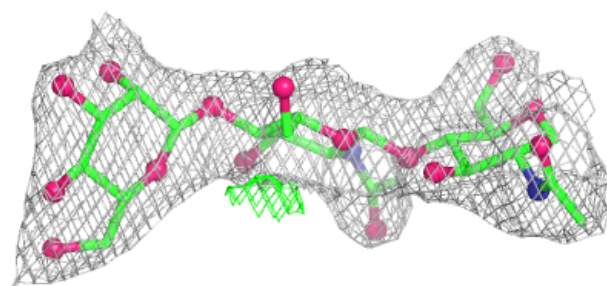
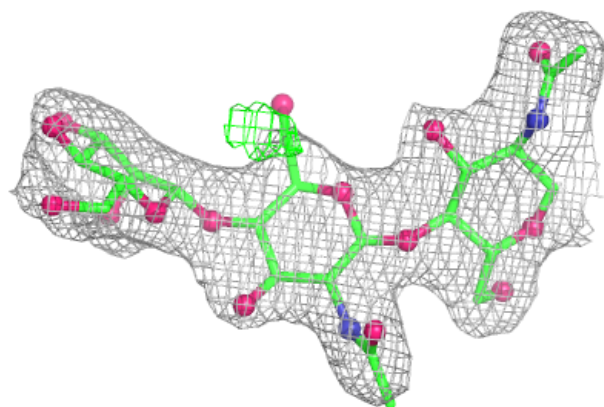
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	C	5	11/12	0.88	0.09	46,62,68,73	0
3	FUC	C	6	10/11	0.88	0.13	58,72,86,86	0
3	NAG	C	1	14/15	0.88	0.11	45,57,66,72	0
4	FUC	E	3	10/11	0.90	0.11	43,51,58,66	0
2	BMA	D	3	11/12	0.91	0.08	57,66,75,79	0
4	NAG	E	1	14/15	0.91	0.09	37,44,53,69	0
3	BMA	C	3	11/12	0.92	0.10	56,72,85,104	0
2	NAG	B	1	14/15	0.93	0.08	32,34,36,43	0
2	NAG	D	1	14/15	0.93	0.08	36,49,54,55	0
3	NAG	C	2	14/15	0.94	0.08	30,52,62,63	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

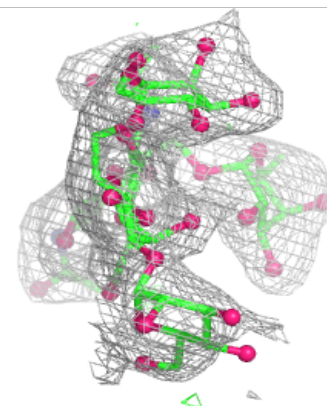
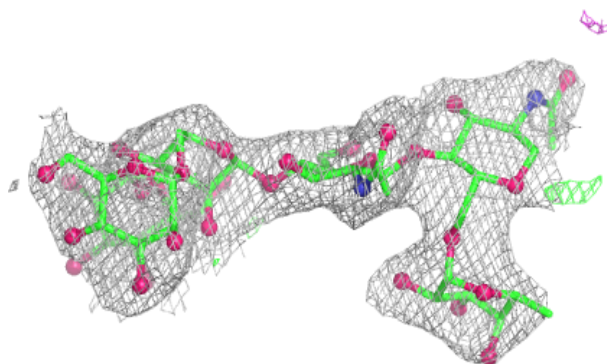
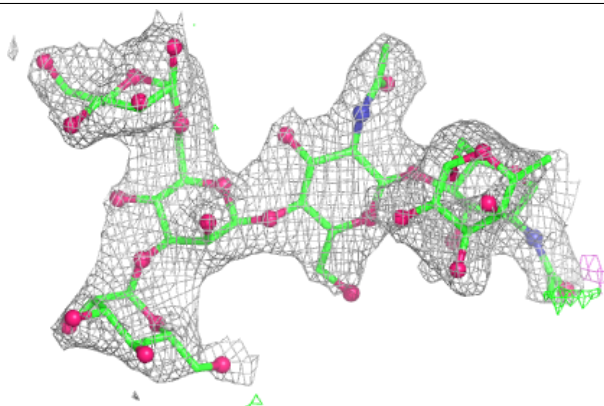


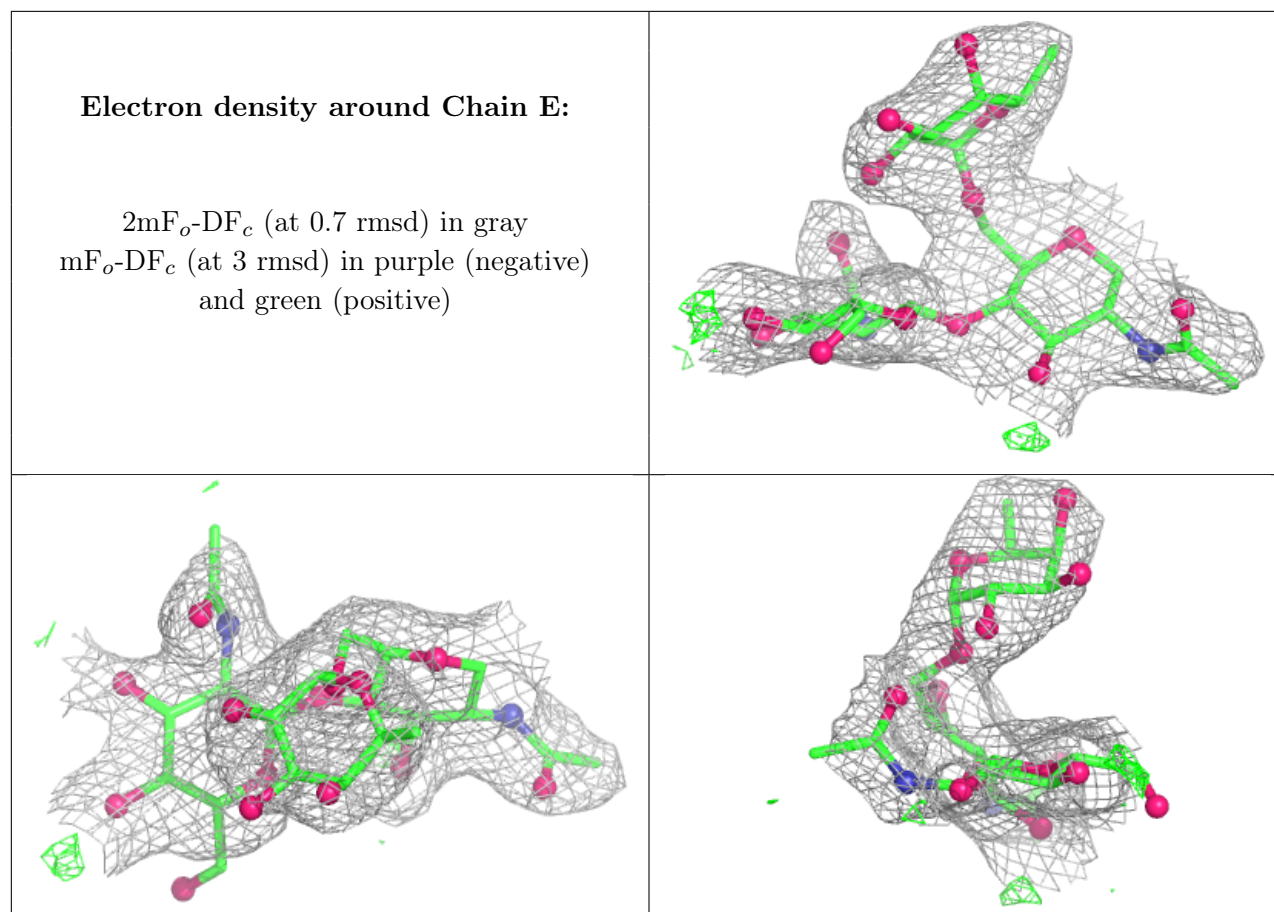
Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain C:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	704	14/15	0.69	0.18	64,78,101,112	0
5	NAG	A	703	14/15	0.73	0.16	49,92,108,115	0
5	NAG	A	702	14/15	0.80	0.14	56,62,70,74	0
6	SO4	A	707	5/5	0.83	0.20	81,84,96,101	0
5	NAG	A	701	14/15	0.88	0.10	42,55,70,70	0
6	SO4	A	708	5/5	0.88	0.14	50,56,75,79	0
6	SO4	A	706	5/5	0.92	0.10	49,51,69,86	0
7	CA	A	709	1/1	0.97	0.05	56,56,56,56	0
6	SO4	A	705	5/5	0.98	0.05	28,30,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.